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COMPUTATIONAL STUDY OF OBLIQUE SHOCK INDUCED DETONATION WAVE STABILIZATION BY DEFLECTION OF WEDGE SURFACE

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ABSTRACT

The Development of supersonic combustor for hypersonic air breathing propulsion devices involves the study of shock-induced combustion. The mechanism intends to minimize the combustor length. The mechanism involves sufficient entropy generated behind Oblique Shock Wave (OSW) and this will ignite the premixed flow of fuel and air just beneath the OSW. Thus an Oblique Detonation Wave (ODW) formed. The formation and stabilization of ODW depend on free stream flow conditions and wedge angle. Free stream mixed flow should provide minimum entropy generation required for the combustion process and wedge angle, normal Mach number one. This condition is called as Chapman–Jouguet (C-J). One of the methods to stabilize the ODW is deflecting the wedge surface to make it parallel to free stream flow conditions. This leads to the interference of ODW with expansion fan and results in stabilization.

The present research paper's objective is to simulate the proof of concept related to stabilization over finite length wedge. Free stream flow consists of stoichiometric mixture of hydrogen (fuel) and air. A near C-J condition free flow considered from literature. Two-dimensional CFD simulations carried using ANSYS CFX, CFD software based on Finite Volume Method. Hexagonal mesh adopted to capture the flow conditions and generated by ICEM CFD, an advanced meshing software. The chemical reactions modeling is based on multi step Jachimowski's finite rate chemistry models.

KEYWORDS: Hypersonic Flows, Hydrogen-Air Mixture, Stochiometric, Chapman-Jouguet, ODW, CFD & Scramjet

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Original Article

INTRODUCTION

Hypersonic air breathing propulsion application for intercontinental or assisted transport for aero space vehicles in atmospheric regimes requires the development of scramjet combustor with reduced length [1]. One of the methods is to develop shock-induced combustion and combustor known as schramjet engine. A combustion process requires minimum activation energy, temperature or entropy generation. Hypersonic flow over wedge induces an OSW. This weak shock is capable of inducing combustion process for reactive gas mixture [2] and thus ODW formed within the maximum distance of 1 mm [3]. The process should sustain to keep combustion stability i.e. ODW has to be stabilized. Perhaps the ODW settle down by the interaction of wedge with reactive gas mixtures under supersonic flow conditions [4, 5]. The ODW generated in accordance with Chapman–Jouguet (C-J) conditions i.e. wedge angle and free stream conditions only stabilized [6].

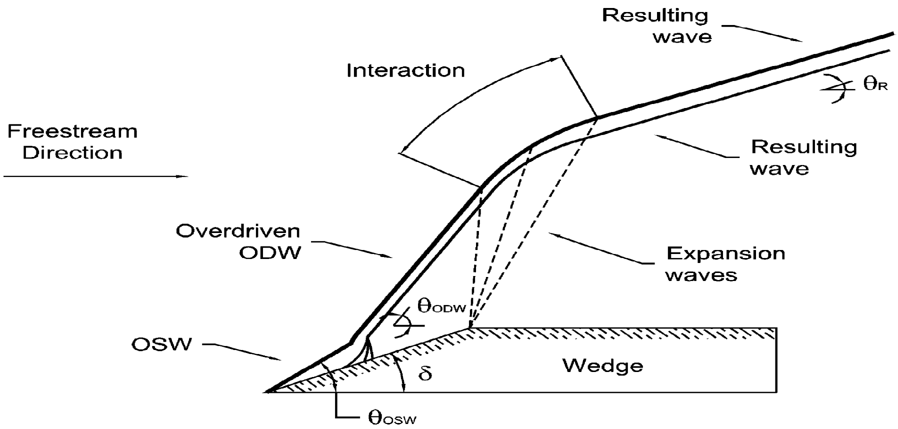

Figure 1: Schematic Presentation of Hypersonic Flow Over Wedge with Featured Angles.

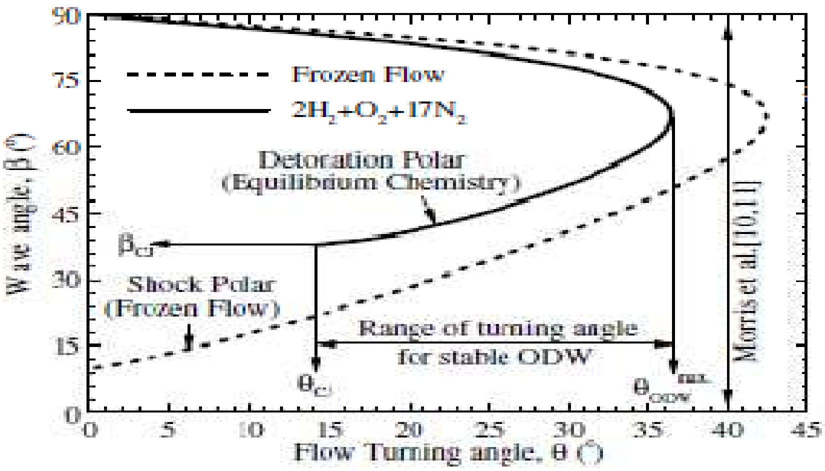

Figure 2: Polar Diagram Representing Analytical Solutions [2].

Interaction of ODW with expansion waves generated at the start of flat surface leads to settling down of ODW. The Schematic of the stabilization mechanism is depicted in Figure 1. An OSW with a wave angle θOSW formed due to hypersonic flow turning over a wedge with an angle δ. This leads to the formation of over driven ODW along the length of the wedge because of the combustion of reactive mixture initiated just behind the OSW. This is indicated by flow deflection i.e. with a large angle, θ_{ODW} that is greater than θ_{OSW}. Further the down stream, overdriven ODW interacts with expansion waves and resulted in a wave whose angle is less than θ_{ODW}. Expansion waves are formed because of a flat surface, which makes flow parallel to free stream. The present research work objective is to prove this concept of ODW stabilization in accordance with C-J conditions.

Figure 2 shows an example of shock polar diagram representing inert gas shock, frozen flow and gas with swift release of energy, free equilibrium chemistry for hydrogen air equivalence reactive mixture with stream conditions, M_∞= 5.55, T_∞= 292K and P_∞= 0.12 bar [7]. ODW is stabilized in the narrow range of flow turning angle as shown in Figure 1, which is reproduced from Jeong et al. [8].

Morris et al. [7], investigated the formation of ODW in three regions of wedge angle, less than θ_{C-J}, in between θ_{C-J} and $\theta_{det,eq}$, above $\theta_{det,eq}$. They gave theoretical predictions based on Rankine–Hugoniot (RH) theory

and detonation polars and showed that a steady, straight ODW may be stabilized only for wedge angles between θ_{C-J} and $\theta_{det,eq}$

Pimentel et al. [9] investigated the possibility of obtaining a CJ ODW by progressive formation of OSW, overdriven ODW and finally C-J ODW. They carried numerical investigation with adaptive mesh technique.

Walter et al., [6] carried numerical simulations to analyze the effect of expansion wave interaction with ODW on the sustainability of ODW over a finite length wedge. They employed C-J conditions, which yields a minimum entropy generation in their simulations. They concluded that the expansion wave generated at the end of the ramp angle weakened the strength of ODW and thus there is a decrease in θ_{ODW}.

Jeong et al. [8] numerically investigated the formation of ODW for wedge angles greater than detachment point. The parameter varied is wedge length to account for different ratios of chemical and fluid time scale. They observed no ignition, oscillatory combustion and detached bow under different time scales.

Honghui Teng et al. [10] numerically simulated ODW to investigate induction zone structures with different incident Mach numbers. They observed three kinds of shock structures observed at the end of the induction zone, which are the k, X and Y-shaped shock.

Liu et al, [11] conducted numerical simulations to check the possibility of ODW stabilization by finite length wedge. They concluded that ODW can be stabilized on a finite-length wedge, whose length is smaller than the induction length of the mixture.

Sudip et al. [12] numerically studied the formation of ODW over a non-uniform dual ramp is to reveal C-J ODW has been explored. They found that near C-J ODW can be formed with dual ramp by reducing induction time.

CFD GOVERNING EQUATIONS AND CHEMICAL KINETICS MECHANISM

Finite Volume Method employed for flow field analysis using ANSYS CFX, CFD software. Two-dimensional simulations are carried with a three-dimensional domain, assuming symmetry boundary condition in Z-direction. Transient simulations are carried out. Timestep in the order of 10-8 is chosen to capture chemical reactions. The maximum courant number is in the order of 5. Radiation heat transfer not considered for the analysis. Molecular transport effects are assumed as nil in the region outside boundary layer on wedge [13]. Conservative form of governing equations of flow is as follows:

Table I: Reaction Mechanism For H2-Air Combustion

	Equation	A [mol/cm^3/s]	n[1]	E [cal/mol]
1	H2 + O2 <=> OH + OH	1.70E13	0.00	48000
2	OH + H2 <=> H2O + H	2.20E13	0.00	5150
3	OH + OH <=> H2O + O	6.30E12	0.00	1090
4	H + O2 <=> OH + O	2.60E14	0.00	16800
5	O + H2 <=> OH + H	1.80E10	1.00	8900
6	H + OH + M <=> H2O + M	2.20E22	-2.00	0.00
7	H + H + M <=> H2 + M	6.40E17	-1.00	0.00
8	H + O + M <=> OH + M	6.00E16	-0.60	0.00
9	H + O2 + M <=> HO2 + M	2.10E15	0.00	-1000
10	HO2 + H <=> H2 + O2	1.30E13	0.00	0.00
11	HO2 + H <=> OH + OH	1.40E14	0.00	1080
12	HO2 + H <=> H2O + O	1.00E13	0.00	1080
13	HO2 + O <=> O2 + OH	1.50E13	0.00	950
14	HO2 + OH <=> H2O + O2	8.00E12	0.00	0.00

Continuity: $\frac{\partial \rho}{\partial t} + \nabla(\emptyset) = 0$ (1)

Momentum: $\frac{\partial(\rho U)}{\partial t} + \nabla(\emptyset U) = 0$ (2)

Energy: $\frac{\partial(\rho E)}{\partial t} + \nabla(\emptyset H) = 0$ (3)

Species: $\frac{\partial(\rho Y_i)}{\partial t} + \nabla(\emptyset Y_i) = \dot{x_i} W_i$ (4)

Where, $E = e + \frac{1}{2}U^2 = \sum_i Y_i e_i$ is total energy;

$H = E + \frac{p}{\rho}$ is the total enthalpy;

Y_i is the mass fraction of the chemical species i;

W_i is the molecular weight of the species i;

$\dot{x_i}$ is the species molar production rate

$\dot{x_i} W_i$ is the reaction source term

State of the equation, $= \rho RT \sum_i \frac{Y_i}{W_i}$, is used in conjunction with above governing equations to define an inviscid reactive flow regime.

The chemical kinetics mechanism for the combustion of H2-air mixture consists of multiple step reactions. The chemical reaction rates are computed incorporating the Arrhenius law:

$k = AT^n exp\left(\frac{-E}{RT}\right)$ (5)

The Detailed kinetic chemical mechanism involves 14 multiple reactions of Hydrogen and Oxygen. Table I shows the coefficients of the reaction rates which are based on Jachimowski et al. [14]. The reaction coefficients are incorporated in ANSYS CFX. The chemical production rates and thermodynamic properties are computed by using ANSYS CFX, CFD software.

Third body efficiencies:

H2O = 6.0 (6)

H2 = 2.0, H2O = 6.0 (7)

H2O = 5.0 (8)

H2 = 2.0, H2O = 16.0 (9)

COMPUTATIONAL METHODOLOGY

The C-J conditions related to the wedge dimensions, turning angle and free stream flow conditions are based on numerical simulations carried by Walter et al[]. A Wedge with a turning angle δ=30° with a height of 2.15 mm is considered. The Length of the wedge with flat surface included is 30-mm. The computational domain with boundary conditions presented in figure 2. The front two surfaces are assigned inlet boundary with supersonic inlet condition, specified velocity and pressure. Free stream flow conditions assigned are: T∞, free stream temperature = 275 K, Pressure = 0.75 atm and Mach Number of 6.83.

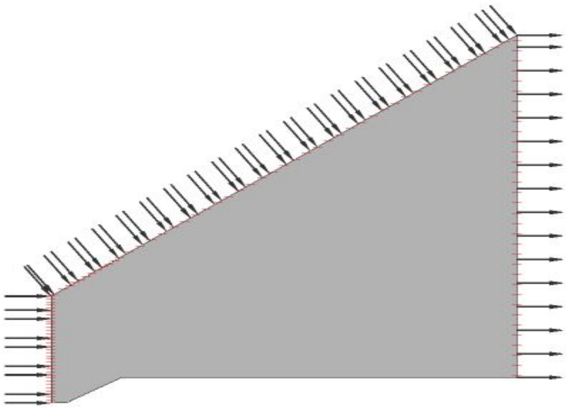

Figure 3: Computational Domain with Boundary Conditions.

The Structured mesh is employed for the computation and the minimum numbers of nodes are ensured along horizontal and vertical direction to capture the shock. The geometry and mesh creation is done using ICEM CFD, advanced meshing software. The Stochiometric flow of H2-Air is considered at the Mach number 6.83. Supersonic outlet conditions imposed at the outlet.

RESULTS AND DISCUSSIONS

Results are presented for the computational simulation of hypersonic flow over a wedge at a Mach number of 6.83 with reactive mixtures (stoichiometric mixture of Hydrogen and Air). Pressure, temperature, Mach number and mass fractions of H, OH & H_2O are presented in the form of contours for overall domain and in the vicinity of expansion corner. The Mach number is based on C-J range of wedge deflection. The wedge length allows the transformation of OSW to ODW and completely over driven ODW. The Inherent structure of the Detonation wave not captured in this analysis and the objective is only to prove the concept of stabilization. Transient simulations with a time step of $5X10^{-8}$ sec carried for a total time of 1.5 sec, which is sufficient for reactive mixture to pass the domain.

Figure 4 presents the variation of the flow field in terms of pressure and temperature contour. It is observed that ODW is inclined up to the end of the inclined ramp and measured ODW angle, $\theta_{ODW} = 58°$ approximately. ODW is bent in shape after the interaction with expansion waves at the end of the inclined ramp. This leads to the reduction of ODW angle to 45° approximately. Inlet static pressure of 0.75 atm is imposed at the inlet boundary and maximum pressure with a value of 34.78 bar is observed just below the OSW wave i.e. in the region of OH formation. This value is in good agreement with analytically evaluated pressure at the Zel'dovich, von Neumann, and Doring (ZND)[33] state by the polar analysis for the C–J ODW with value of 32.1 atm. The maximum temperature computed is 4011 K in the region below the ODW and above the inclined ramp.

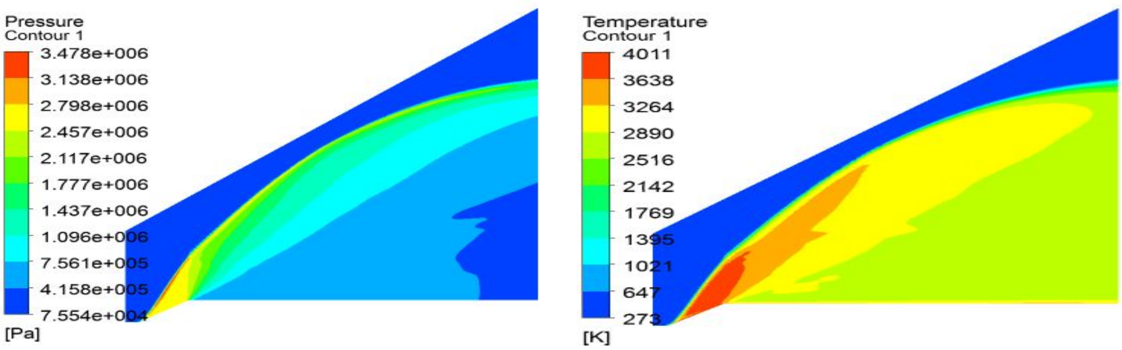

Figure 4: Pressure and Temperature Contour for the Entire Domain.

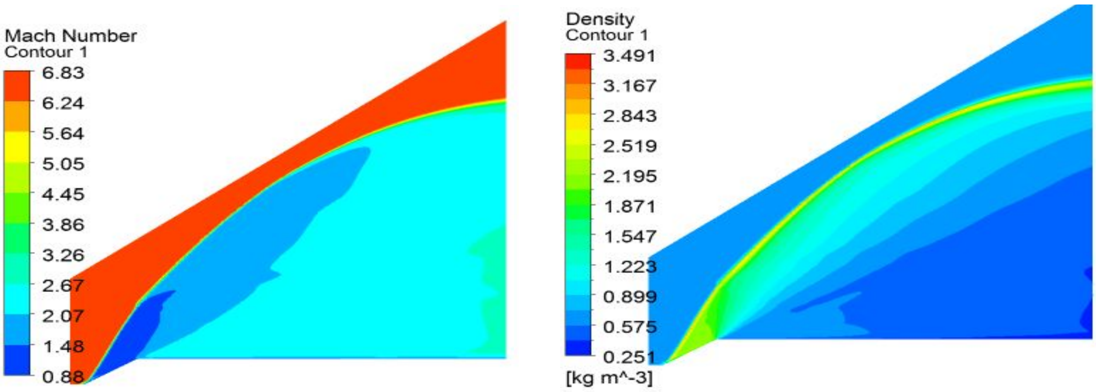

Figure 5: Mach Number and Density Contour for Entire Domain.

Figure 5 represents the Mach number and density contour for the entire flow field. Inlet Mach number imposed is 6.83. The Flow structure is explained above. Density jump is observed just below the ODW. Expansion waves are observed at the beginning of flat surface.

Figure 6 shows the contours of pressure and temperature flow field near the transition region i.e. at the start of flat surface. Expansion waves can be observed at the ramp end. Interaction of ODW with expansion waves can be observed, which is indicated by abrupt end of maximum presuure line (red colour just beneath the ODW).

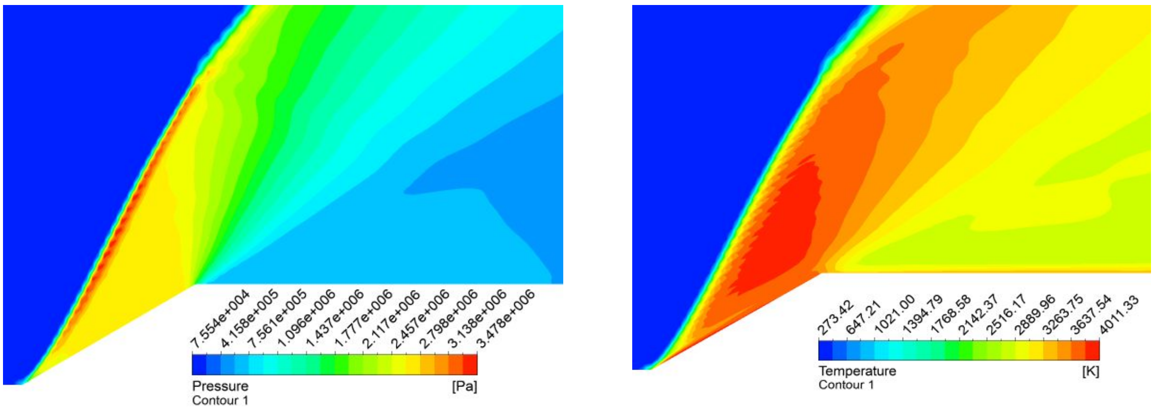

Figure 6: Pressure and Temperature Contour Near the Transition Region.

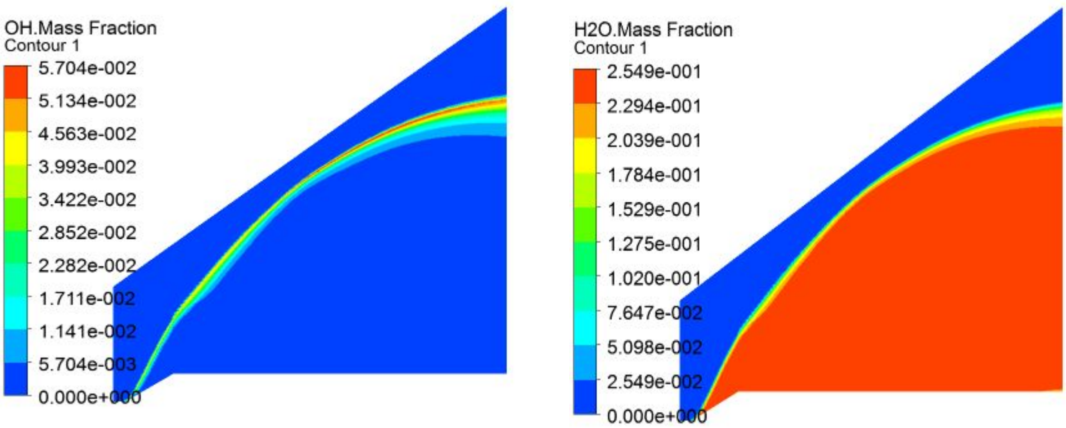

Figure 7: Mass Fraction Contour of OH and H2O Species.

Figure 7 shows the mass fraction contour of OH and H2O species. OH variation is observed just in a narrow region below the ODW. The region is increased in width just after the interaction with expansion wave. The maximum water vapor mass fraction computed is 0.2549, which is occupied the entire region between ODW and ramp.

CONCLUSIONS

- Oblique Detonation Wave resulted from the combustion of Hydrogen gas with Air initiated by OSW is captured.
- The maximum pressure obtained is 34 atm just along the ODW upto transition region. This value is in good agreement with analytically evaluated pressure at the Zel'dovich, von Neumann, and D¨oring (ZND) state by the polar analysis for the C–J ODW with value of 32.1 atm.
- The computed value of angle for ODW is 58° and reduction in angle is 9° due to the interaction of ODW with expansion wave.

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